Statistical mechanics and Vlasov equation allow for a simplified hamiltonian description of single pass free electron laser saturated dynamics

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A reduced Hamiltonian formulation to reproduce the saturated regime of a Single Pass Free Electron Laser, around perfect tuning, is here discussed. Asymptotically, N_m particles are found to organize in a dense cluster, that evolves as an individual massive unit. The remaining particles fill the surrounding uniform sea, spanning a finite portion of phase space, approximately delimited by the average momenta ω_+ and ω_-. These quantities enter the model as external parameters, which can be self-consistently determined within the proposed theoretical framework. To this aim, we make use of a statistical mechanics treatment of the Vlasov equation, that governs the initial amplification process. Simulations of the reduced dynamics are shown to successfully capture the oscillating regime observed within the original N-body picture.

I. GENERAL BACKGROUND

Free-Electron Lasers (FELs) are coherent and tunable radiation sources, which differ from conventional lasers in using a relativistic electron beam as their lasing medium, hence the term free-electron.

The physical mechanism responsible for the light emission and amplification is the interaction between the relativistic electron beam, a magnetostatic periodic field generated in the undulator and an optical wave copropagating with the electrons. Due to the effect of the magnetic field, the electrons are forced to follow sinusoidal trajectories, thus emitting synchrotron radiation. This *spontaneous emission* is then amplified along the undulator until the laser effect is reached. Among different schemes, single-pass high-gain FELs are currently attracting growing interest, as they are promising sources of powerful and coherent light in the UV and X ranges. Besides the Self Amplified Spontaneous Emission (SASE) setting [1], seeding schemes may be adopted where a small laser signal is injected at the entrance of the undulator and guides the subsequent amplification process [2]. In the following we shall refer to the latter case. Basic features of the system dynamics are successfully captured by a simple one-dimensional Hamiltonian model [15] introduced by Bonifacio and collaborators in [3]. Remarkably, this simplified formulation applies to other physical systems, provided a formal translation of the variables involved is performed. As an example, focus on kinetic plasma turbulence, e.g. the electron beam-plasma instability. When a weak electron beam is injected into a thermal plasma, electrostatic modes at the plasma frequency (Langmuir modes) are destabilized. The interaction of the Langmuir waves and the electrons constituting the beam can be studied in the framework of a self-consistent Hamiltonian picture [4], formally equivalent to the one in [3]. In a recent paper [5] we established a bridge between these two areas of investigation (FEL and plasma), and exploited the connection to derive a reduced Hamiltonian model to characterize the saturated dynamics of the laser. According to this scenario, N_m particles are trapped in the resonance, i.e. experience a bouncing motion in one of the (periodically repeated) potential wells, and form a clump that evolves as a single macro-particle localized in space. The remaining particles populate the surrounding halo, being almost uniformly distributed in phase space between two sharp boundaries, whose average momentum is labeled ω_+ and ω_-. The issue of providing a self-consistent estimate for the external parameters N_m, ω_+ and ω_- is addressed and solved in this paper.

This long-standing problem was first pointed out by Tennyson et al. in the pioneering work [6] and recently revisited in [4]. A first attempt to calculate N_m is made in [9] where a semi-analytical argument is proposed. In this respect, the strategy here proposed applies to a large class of phenomena whose dynamics can be modeled within a Hamiltonian framework [4, 7] displaying the emergence of collective behaviour [8].

The paper is organized as follows. In Section II we introduce the one-dimensional model of a FEL amplifier [3] and review the derivation of the reduced Hamiltonian [5, 6]. Section III recalls the statistical mechanics approach to estimate the saturated laser regime. In Sections IV to VI the analytic characterization of N_m, ω_+ and ω_- is given in details and the results are then tested numerically in section VII. Finally, in Section VIII we sum up and draw our conclusions.

II. FROM THE SELF-CONSISTENT N-BODY HAMILTONIAN TO THE REDUCED FORMULATION

Under the hypothesis of one-dimensional motion and monochromatic radiation, the steady state dynamics of a Single-Pass Free Electron Laser is described by the following set of equations:

$$\frac{\mathrm{d}\theta_j}{\mathrm{d}\bar{z}} = p_j \quad , \tag{1}$$

$$\frac{\mathrm{d}p_j}{\mathrm{d}\bar{z}} = -Ae^{i\theta_j} - A^* e^{-i\theta_j} \quad , \tag{2}$$

$$\frac{\mathrm{d}A}{\mathrm{d}\bar{z}} = i\delta A + \frac{1}{N}\sum_j e^{-i\theta_j} \quad , \tag{3}$$

where $\bar{z} = 2k_w \rho z \gamma_r^2/\langle\gamma\rangle_0^2$ is the rescaled longitudinal coordinate, which plays the role of time. Here, $\rho = [a_w \omega_p/(4ck_w)]^{2/3}/\gamma_r$ is the so-called Pierce parameter, $\langle\gamma\rangle_0$ the mean energy of the electrons at the undulator's entrance, $k_w = 2\pi/\lambda_w$ the wave number of the undulator, $\omega_p = (4\pi e^2 n/m)^{1/2}$ the plasma frequency, c the speed of light, n the total electron number density, e and m respectively the charge and mass of one electron. Further, $a_w = eB_w/(k_w mc^2)$, where B_w is the rms peak undulator field. Here $\gamma_r = \left(\lambda_w(1+a_w^2)/2\lambda\right)^{1/2}$ is the resonant energy, λ_w and λ being respectively the period of the undulator and the wavelength of the radiation field. Introducing the wavenumber k of the FEL radiation, the two canonically conjugated variables are (θ, p), defined as $\theta = (k+k_w)z - 2\delta\rho k_w z\gamma_r^2/\langle\gamma\rangle_0^2$ and $p = (\gamma - \langle\gamma\rangle_0)/(\rho\langle\gamma\rangle_0)$. θ corresponds to the phase of the electrons with respect to the ponderomotive wave. The complex amplitude $A = A_x + iA_y$ represents the scaled field, transversal to z. Finally, the detuning parameter is given by $\delta = (\langle\gamma\rangle_0^2 - \gamma_r^2)/(2\rho\gamma_r^2)$, and measures the average relative deviation from the resonance condition.

The above system of equations (N being the number of electrons) can be derived from the Hamiltonian

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2} - \delta I + 2\sqrt{\frac{I}{N}} \sum_{j=1}^{N} \sin(\theta_j - \varphi), \tag{4}$$

where the intensity I and the phase φ of the wave are given by $A = \sqrt{I/N}\exp(-i\varphi)$. Here the canonically conjugated variables are (p_j, θ_j) for $1 \le j \le N$ and (I, φ). Besides the "energy" H, the total momentum $P = \sum_j p_j + I$ is also conserved. By exploiting these conserved quantities, one can recast the FEL equations of motion in the following form for the set of $2N$ conjugate variables (q_j, p_j) [10]:

$$\dot{q_j} = p_j - \frac{1}{\sqrt{NI}} \sum_{l=1}^{N} \sin q_l + \delta \ , \tag{5}$$

$$\dot{p_j} = -2\sqrt{\frac{I}{N}} \cos q_j, \tag{6}$$

where the dot denotes derivation with respect to $\bar{z}$, and $q_j = \theta_j - \varphi \ \mathrm{mod}(2\pi)$ is the phase of the j^{th} electron in a proper reference frame. The fixed points of system (5)-(6) are determined by imposing $\dot{q_j} = \dot{p_j} = 0$ and solving:

$$p_j - \frac{1}{\sqrt{NI}} \sum_{l=1}^{N} \sin q_l + \delta = 0 \ , \tag{7}$$

$$2\sqrt{\frac{I}{N}} \cos q_j = 0. \tag{8}$$

An elliptical fixed point is found for $q_i = \bar{q} = 3\pi/2$. The conjugate momentum solves $(\bar{p} + \delta)\sqrt{P/N - \bar{p}} + 1 = 0$ and therefore depends on P/N. We shall return on this issue in the following Sections.

For a monokinetic initial beam with velocity resonant with the wave, equations (1), (2) and (3) predict an exponential instability and a late oscillating saturation for the amplitude of the radiation field. Numerical simulations fully confirm this scenario as displayed in fig. 1. In the single particle (q,p) space, a dense core of particles is trapped by the wave and behaves like a large "macro-particle", that evolves coherently in the resonance. The distances between these particles do not grow exponentially fast (as is the case for chaotic motion) but grow at most linearly with time (for particles trapped in the resonance with different adiabatic invariants, i.e.essentially different action in the single particle pendulum-like description). This linear-in-time departure of the particles appears in the differential rotation in fig. 2, while the remaining particles are almost uniformly distributed between two oscillating boundaries. Having observed the formation of such structures in the phase-space allowed to derive a simplified Hamiltonian model to characterize the asymptotic evolution of the laser [5, 6]. This reduced formulation consists in only four degrees of freedom, namely the wave, the macro-particle and the two boundaries delimiting the portion of space occupied by the so-called *chaotic sea*, i.e. the uniform halo surrounding the inner core.

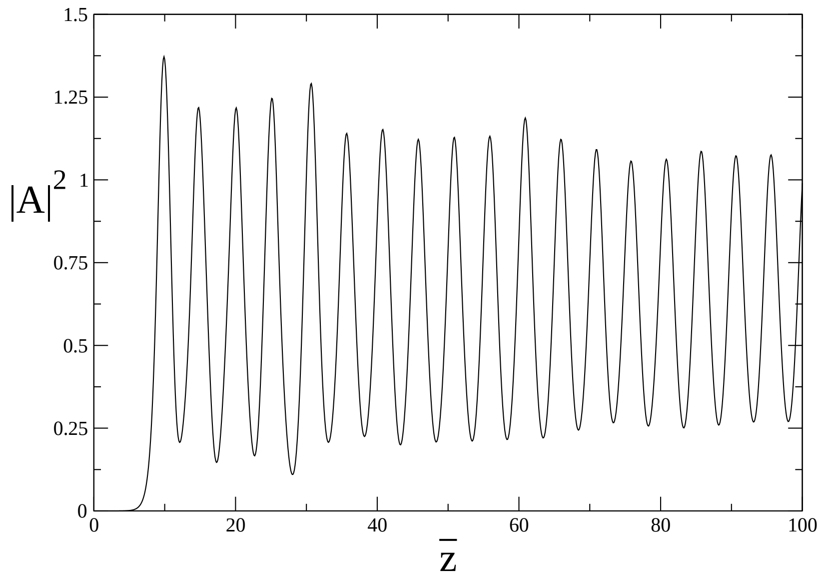

FIG. 1: *Evolution of the radiation intensity as follows from equations (1), (2) and (3). $N = 10^4$ electrons are simulated, for an initial mono-energetic profile. Here $\delta = 0$ and $I(0) \simeq 0$. Particles are initially uniformly distributed in space.*

In [5] we hypothesized the macro-particle to be formed by N_m individual massive units, and introduced the variables (ζ, ξ) to label its position in the phase space.

The $N_c = N - N_m$ particles of the surrounding halo are treated as a *continuum* with constant phase space distribution, $f_{sea}(\theta, p, \bar{z}) = f_c$, between two boundaries, namely $p_+(\theta, \bar{z})$ and $p_-(\theta, \bar{z})$ such that:

$$p_\pm = p_\pm^0 + \widetilde{p}_\pm \exp(i\theta) + \widetilde{p}_\pm^* \exp(-i\theta) \ , \tag{9}$$

where $p_\pm^0$ represents their mean velocity. These assumptions allow to map the original system, after linearizing with respect to $\widetilde{p}_\pm$, into [5]:

$$\begin{aligned} \ddot{\zeta} &= i\Phi e^{i\zeta} - i\Phi^* e^{-i\zeta} && (10) \\ \frac{1}{2}\dot{V}_\pm &= -\frac{i}{2}\omega_\pm V_\pm + i\Phi && (11) \\ \dot{\Phi} &= \frac{i}{2}\frac{N_c}{N}\frac{V_+ - V_-}{\omega_+ - \omega_-} + i\frac{N_m}{N}e^{-i\zeta} + i\delta\Phi && (12) \end{aligned}$$

where [16]

$$
\begin{aligned}
A &= -i\Phi && (13)\\
\widetilde{p}_\pm &= V_\pm/2 && (14)\\
\widetilde{p}^0_\pm &= \omega_\pm && (15)
\end{aligned}
$$

Normalizing the density in the chaotic sea to unity yields $f_c = 1/(2\pi\Delta\omega)$, where $\Delta\omega := \omega_+ - \omega_-$ represents the (average) width of the chaotic sea. The above system can be cast in a Hamiltonian form by introducing new actions $I_\pm$ and their conjugate angles $\varphi_\pm$:

$$
\begin{aligned}
V_+ &= \sqrt{4\frac{I_+\Delta\omega}{N_c}}e^{-i\varphi_+} && (16)\\
V_- &= \sqrt{4\frac{I_-\Delta\omega}{N_c}}e^{i\varphi_-}. && (17)
\end{aligned}
$$

A pictorial representation of the main quantities involved in the analysis is displayed in fig. 3. In addition:

$$
\Phi = iA = -\sqrt{\frac{I}{N}}e^{-i(\varphi+\frac{\pi}{2})}. \tag{18}
$$

The reduced 4-degrees-of-freedom Hamiltonian reads, up to a constant irrelevant to the evolution equations:

$$
H_4 = \frac{\xi^2}{2N_m} - \delta I + \omega_+ I_+ - \omega_- I_- - 2\alpha\left[\sqrt{II_+}\sin(\varphi-\varphi_+) - \sqrt{II_-}\sin(\varphi+\varphi_-)\right] - 2\beta\sqrt{I}\sin(\varphi-\zeta), \tag{19}
$$

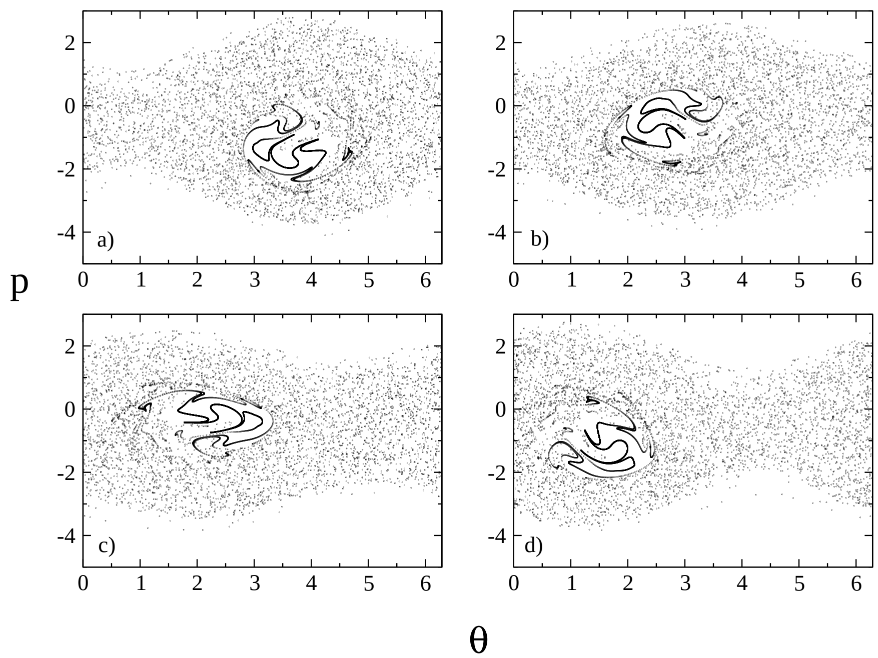

FIG. 2: *Phase space portraits for different position along the undulator [$\bar{z}$ = a) 80, b) 81, c) 83, d) 84]. The differential rotation of the macro-particle is clearly displayed. For the parameters choice refer to the caption of Fig. 1.*

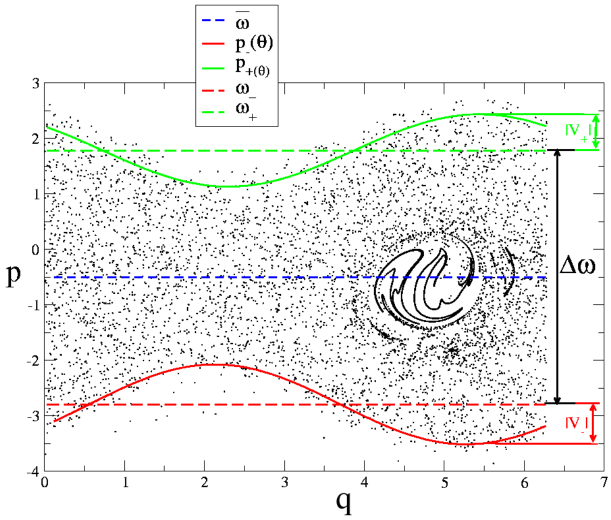

FIG. 3: *(q,p) phase space portrait in the deep saturated regime for a monokinetic initial beam ($I(0) \simeq 0$, $p_j(0) = 0$ and q uniformly distributed in $[0, 2\pi]$). The two solid lines result from a numerical fit performed according to the following strategy. First, the particles located close to the outer boundaries are selected and then the expression $p_\pm(q) = \omega_\pm \mp |V_\pm| \sin(q + B_\pm)$ is numerically adjusted to interpolate their distribution. Here, $|V_\pm|$, $B_\pm$ and $\omega_\pm$ are free parameters. The numerics are compatible with the simplifying assumption $B_+ = B_- \simeq 0$.*

where

$$\alpha = \sqrt{\frac{N_c}{N\Delta\omega}} \tag{20}$$

$$\beta = \frac{N_m}{\sqrt{N}} \tag{21}$$

The first four terms represent the kinetic energy of the macro-particle, the oscillation of the wave and the harmonic contributions associated to the oscillation of the chaotic sea boundaries. The remaining terms refer to the interaction energy. Total momentum is $P = \xi + I + N_c\bar{\omega}$. The Hamiltonian (19) allows for a simplified description of the late nonlinear regime of the instability, provided the three parameters ω_+, ω_- and N_m are given.

To achieve a complete and satisfying theoretical description we need to provide an argument to self-consistently estimate these coefficients. To this end, we shall use the analytical characterization of the asymptotic behavior of the laser intensity and beam bunching (a measure of the electrons spatial modulation) obtained in [11] with a statistical mechanics approach. In the next section these results are shortly reviewed.

III. STATISTICAL THEORY OF SINGLE-PASS FEL SATURATED REGIME

As observed in the previous Section, the process of wave amplification occurs in two steps: an initial exponential growth followed by a relaxation towards a quasi-stationary state characterized by large oscillations. This regime is governed by the Vlasov equation, rigorously obtained by performing the continuum limit ($N \to \infty$ at fixed volume and energy per particle) [4, 11, 12] on the discrete system (1-3). Formally, the following Vlasov-wave system is found:

$$\frac{\partial f}{\partial \bar{z}} = -p\frac{\partial f}{\partial \theta} + 2(A_x \cos\theta - A_y \sin\theta)\frac{\partial f}{\partial p} \quad , \tag{22}$$

$$\frac{dA_x}{d\bar{z}} = -\delta A_y + \int f \cos\theta \, \mathrm{d}\theta \, \mathrm{d}p \quad , \tag{23}$$

$$\frac{dA_y}{d\bar{z}} = \delta A_x - \int f \sin\theta \, \mathrm{d}\theta \, \mathrm{d}p \quad . \tag{24}$$

The latter conserves the pseudo-energy per particle

$$\epsilon = \int \frac{p^2}{2} f(\theta, p)\,\mathrm{d}\theta\,\mathrm{d}p - \delta(A_x^2 + A_y^2) + 2\int (A_x \sin\theta + A_y \cos\theta) f(\theta, p)\,\mathrm{d}\theta\,\mathrm{d}p \tag{25}$$

and the momentum per particle

$$\sigma = \int p f(\theta, p)\,\mathrm{d}\theta\,\mathrm{d}p + (A_x^2 + A_y^2)\ . \tag{26}$$

A subsequent slow relaxation towards the Boltzmann equilibrium is observed. This is a typical finite-N effect and occurs on time-scales much longer than the transit trough the undulator [3, 4, 13]. For our calculations we are interested in the first saturated state. To estimate analytically the average intensity and bunching parameter in this regime we exploit the statistical treatment of the Vlasov equation, presented in [11]. In the following, we provide a short outline of the strategy. Since the Gibbs ensembles are equivalent for this model, note that the same expressions are recovered through a canonical calculation [4, 11, 14].

The basic idea is to coarse-grain the microscopic one-particle distribution function $f(\theta, p, \bar{z})$. An entropy is then associated to the coarse-grained distribution $\bar{f}$, which essentially counts a number of microscopic configurations. Neglecting the contribution of the field, since it represents only one degree of freedom within the $(N+1)$ of the Hamiltonian (4), one assumes

$$s(\bar{f}) = -\int \left[\frac{\bar{f}}{f_0}\ln\frac{\bar{f}}{f_0} + \left(1 - \frac{\bar{f}}{f_0}\right)\ln\left(1 - \frac{\bar{f}}{f_0}\right)\right] f_0 \mathrm{d}\theta\,\mathrm{d}p \simeq -\int \left[\frac{\bar{f}}{f_0}\ln\frac{\bar{f}}{f_0}\right] f_0 \mathrm{d}\theta \mathrm{d}p\ , \tag{27}$$

where the constant f_0 is related to the initial distribution [17].

The equilibrium is computed by maximizing this entropy, while imposing the dynamical constraints. This corresponds to solving the constrained variational problem

$$S(\epsilon, \sigma) = \max_{\bar{f}, A_x, A_y}\left(s(\bar{f})\Big| H(\bar{f}, A_x, A_y) = N\epsilon; P(\bar{f}, A_x, A_y) = N\sigma; \int f(\theta, p)\,\mathrm{d}\theta\,\mathrm{d}p = 1\right), \tag{28}$$

which leads to the equilibrium values

$$\bar{f} = f_0 \frac{e^{-\beta(p^2/2 + 2A\sin\theta) - \lambda p - \mu}}{1 + e^{-\beta(p^2/2 + 2A\sin\theta) - \lambda p - \mu}} \tag{29}$$

$$A = \sqrt{A_x^2 + A_y^2} = \frac{\beta}{\beta\delta - \lambda}\int \sin(\theta)\bar{f}(\theta, p)\,\mathrm{d}\theta\,\mathrm{d}p, \tag{30}$$

where β, λ and μ are the Lagrange multipliers for the energy, momentum and normalization constraints and, in addition, we have assumed the non-restrictive condition $\sum\cos(\theta_i) = 0$ [11]. Using then the three equations for the constraints, the statistical equilibrium calculation is reduced to finding the values of the multipliers as functions of energy ϵ and momentum σ. These equations lead directly to the estimates of the equilibrium values for the intensity I and bunching parameter $b = |\sum\exp(i\theta_i)|/N$.

In the following, we focus on the case of an initially monokinetic beam injected at the wave velocity, while the initial wave intensity is negligible, so that $\epsilon = 0$ and $\sigma = 0$. Moreover we let $f_0 \to \infty$, which amounts to $\mu \to \infty$ in eq. (29). Results are displayed in fig. 4 showing remarkably good agreement between theory and simulations, below the critical threshold $\delta_c \simeq 1.9$ that marks the transition between high and low gain regimes. This transition is purely dynamical and cannot be reproduced by the statistical calculation.

Analytically, it turns out that

$$b = |A|^3 - |A|\delta = \frac{\mathrm{I}_1(2/(3|A|^3 - 2\delta|A|))}{\mathrm{I}_0(2/(3|A|^3 - 2\delta|A|))} \tag{31}$$

where I_n is the modified Bessel function of order n. In particular for $\delta = 0$, one finds $|A|^2 = I/N \simeq 0.65$ and $b \simeq 0.54$.